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A Technical Description of the NAVDAS Adjoint System

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14. ABSTRACT
This report provides a technical description of the adjoint code for the NRL Atmospheric Variational Data Assimilation System (NAVDAS). The output of the NAVDAS adjoint is an array that contains the sensitivity of a user-defined forecast costfunction with respect to the complete set of observations assimilated by NAVDAS at a particular time. The input for the NAVDAS adjoint is an analysis sensitivity vector provided by the adjoint of a forecast model such as NOGAPS. Step by step guidelines for using the NAVDAS adjoint system to compute observation sensitivity are given. The basic theory of observation sensitivity is outlined, and features of the adjoint code and main subroutines are described in detail. Examples of observation sensitivity applications are provided, including the impact of innovations on short-range forecast error, and targeted observing.

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Contents

A TECHNICAL DESCRIPTION OF THE NAVDAS ADJOINT SYSTEM

1 Introduction

Adjoint versions of atmospheric forecast models have been developed and applied, beginning in the mid 1980s, to a wide variety of applications in numerical weather prediction, including data assimilation, sensitivity studies, singular vector generation and targeted (or adaptive) observing. The literature describing adjoint methods in numerical weather prediction is now quite extensive, and a few selected papers on these topics include Talagrand and Courtier (1987), Buizza et al. (1993), Langland et al. (1995), Rabier et al (1996), Errico (1997), Gelaro et al. (1998), Palmer et al. (1998), Bergot et al. (1999), Langland et al. (2002), Bergot and Doerenbecher (2002), and Leutbecher et al. (2002). More recently, it has been shown (Baker and Daley 2000) that the adjoint of a *data assimilation procedure* can be used to provide the sensitivity of a forecast costfunction to the observations and background in an atmospheric analysis. This extension of adjoint sensitivity methods into observation space is a significant advance in efforts to understand factors that control atmospheric predictability and to improve data assimilation procedures.

The first version of the NAVDAS (NRL Atmospheric Variational Data Assimilation System) adjoint was developed by Roger Daley during 1999-2000 and is briefly described in Daley and Barker (2001). This code was used for the Ph.D. research of Nancy Baker (Baker 2000, Baker and Daley 2000) and for preliminary observation sensitivity tests by Rolf Langland. However, substantial revisions to the regular

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(forward) NAVDAS code between 2000 and 2002 made it necessary to develop a new version of the adjoint, and a code development project was therefore initiated in 2002. The current NAVDAS adjoint was primarily developed from a version of NAVDAS obtained on June 18, 2002. It is a completely new adjoint code, although based on the framework of the original Daley version. Since NAVDAS is a linear procedure, there is no separate tangent linear version of NAVDAS, and the adjoint was developed line by line directly from the regular NAVDAS Fortran code. The NAVDAS adjoint code was further updated by the authors using NAVDAS code obtained in March 2003 and January 2004 that included modifications to background error covariance, radiance assimilation, and other changes. This report provides the first complete description of the NAVDAS adjoint, including observation sensitivity equations and overview of the Fortran code (Section 2), steps involved in running and verifying the adjoint code (Section 3), and examples of observation sensitivity applications (Section 4).

2 NAVDAS Adjoint Development

2.1 Observation Sensitivity

The basic purpose of the NAVDAS adjoint is to provide the sensitivity of a user-defined scalar costfunction[1] J with respect to the vector of observations $\mathbf{y}$ used by

[1] J can be any differentiable function of the forecast model variables, such as forecast error, vorticity, surface pressure, temperature, wind speed, etc.

NAVDAS in its assimilation procedure. The costfunction J is a function of a model forecast ($\mathbf{x}_f$) started from an analyzed initial condition ($\mathbf{x}_a$) and J may also be referred to as a "forecast response function" or "forecast aspect." The "observation sensitivity" vector $\partial J \ / \ \partial \mathbf{y}$ is a gradient in "observation space", e.g., its elements exist at the locations of observations, and it is defined by

$$\frac{\partial J}{\partial \mathbf{y}} = \mathbf{K^T} \frac{\partial J}{\partial \mathbf{x}_a}, \tag{1}$$

where $\partial J \ / \ \partial \mathbf{x}_a$ is an analysis (initial condition) sensitivity gradient provided by the adjoint of a forecast model such as NOGAPS (Rosmond 1997, Hogan et al. 1999). The adjoint operator $\mathbf{K^T} = [\mathbf{HP}_b\mathbf{H^T} + \mathbf{R}]^{-1}\mathbf{HP}_b$ is the transpose of the Kalman gain operator, defined by $\mathbf{K} = \mathbf{P}_b\mathbf{H^T} \ [\mathbf{HP}_b\mathbf{H^T} + \mathbf{R}]^{-1}$ that represents the regular (forward) NAVDAS procedure (Daley and Barker 2001). Note that $[\mathbf{HP}_b\mathbf{H^T} + \mathbf{R}]^{-1}$ is self-adjoint. $\mathbf{H}$ is a linearized operator used to project from gridpoint to observation space, and $\mathbf{P}_b$ and $\mathbf{R}$ are the background and observation error covariance matrices, respectively. The main components of the observation sensitivity calculation are outlined in Fig. 1

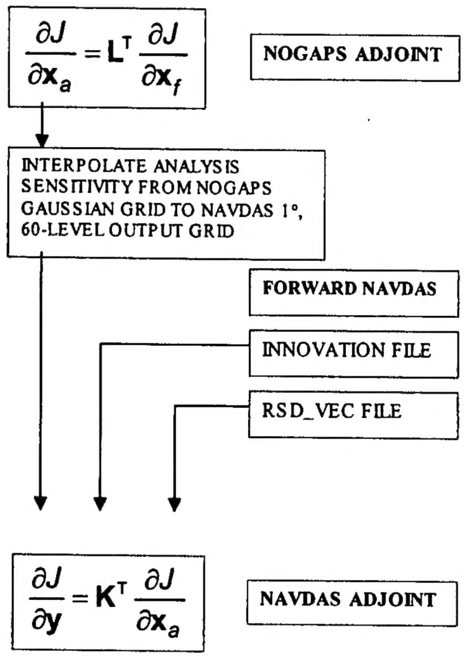

Figure 1: Components of the observation sensitivity calculation using adjoint versions of NOGAPS and NAVDAS, where $\mathbf{L}^T$ is the tangent propagator of NOGAPS, $\mathbf{x}_f$ is the forecast state vector and $\mathbf{x}_a$ is the analysis state vector. Other symbols are defined in Section 2.1.

The initial condition sensitivity is defined by

$$\frac{\partial J}{\partial \mathbf{x}_a} = \mathbf{L}^{\mathbf{T}} \frac{\partial J}{\partial \mathbf{x}_f}, \tag{2}$$

where $\mathbf{L}^{\mathbf{T}}$ is the adjoint (transpose) of the tangent linear propagator $\mathbf{L}$ of the forecast model. Since the Kalman gain operator in NAVDAS is linear, the calculation of sensitivity using (1) is exact. However, calculation of the analysis sensitivity $\partial J \,/\, \partial \mathbf{x}_a$

by the NOGAPS adjoint (2) involves tangent linear approximations and this limits the useful quantitative application of observation sensitivity to short-range forecasts of approximately three days or less. In addition, the current versions of the NOGAPS and NAVDAS adjoints do not include consideration of moist processes or moisture observations, which can be an important limitation in some applications.

A perturbation of the initial conditions $\delta \mathbf{x}_a$ can be propagated to the forecast time by

$$\delta \mathbf{x}_f = \mathbf{L} \delta \mathbf{x}_a \ . \tag{3}$$

The introduction of $\delta \mathbf{x}_a$ changes the scalar costfunction by an amount δJ, which is a function of $\delta \mathbf{x}_f$

$$J + \delta J = f \ (\mathbf{x}_f + \delta \mathbf{x}_f) \tag{4}$$

$$\delta J = f \ (\delta \mathbf{x}_f) = f \ (\mathbf{L} \delta \mathbf{x}_a) \ . \tag{5}$$

Since δJ is a function of $\delta \mathbf{x}_a$, we can extend the definition of the sensitivity gradient in terms of the observation and background used by the data assimilation procedure. The basic linear form of the NAVDAS analysis can be written as

$$\mathbf{x}_a = \mathbf{x}_b + \mathbf{K} \ (\mathbf{y} - \mathbf{H} \mathbf{x}_b) \ , \tag{6}$$

where $\mathbf{x}_b$ is a background forecast. In the regular form of NAVDAS (Daley and Barker, 2001) the operator $\mathbf{H}$ may be nonlinear for some types of observations. If we

perturb the observations by $\delta\mathbf{y}$, then

$$\mathbf{x}_a + \delta\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}\ \ (\mathbf{y}{+}\delta\mathbf{y} - \mathbf{H}\mathbf{x}_b)\ \ . \tag{7}$$

The adjoint of (7), which defines the sensitivity to observations, is (1). However, if we instead perturb the background by $\delta\mathbf{x}_b$, then

$$\mathbf{x}_a + \delta\mathbf{x}_a = (\mathbf{x}_b + \delta\mathbf{x}_b) + \mathbf{K}\ \ (\mathbf{y} - \mathbf{H}\mathbf{x}_b - \mathbf{H}\delta\mathbf{x}_b)\ \ . \tag{8}$$

The adjoint of (8), which defines the sensitivity to the background, has two terms

$$\frac{\partial J}{\partial \mathbf{x}_b} = \frac{\partial J}{\partial \mathbf{x}_a} - \mathbf{H}^{\mathbf{T}}\,\mathbf{K}^{\mathbf{T}}\,\frac{\partial J}{\partial \mathbf{x}_a}\ . \tag{9}$$

In (9), $\mathbf{K}^{\mathbf{T}}\ \partial J\ /\ \partial\mathbf{x}_a$ is the observation sensitivity. Therefore we may re-write (9) as

$$\frac{\partial J}{\partial \mathbf{x}_b} = \frac{\partial J}{\partial \mathbf{x}_a} - \mathbf{H}^{\mathbf{T}}\,\frac{\partial J}{\partial \mathbf{y}}\ , \tag{10}$$

which is an equation for the sensitivity of J to the background in gridpoint space. If there are no observations, it is clear that $\partial J\ /\ \partial\mathbf{x}_b = \partial J\ /\ \partial\mathbf{x}_a$ because the analysis $\mathbf{x}_a$ is then simply the background $\mathbf{x}_b$ carried forward with no change and $\partial J\ /\ \partial\mathbf{y} = \mathbf{0}$. The operator $\mathbf{H}^{\mathbf{T}}$, which is required to project $\partial J\ /\ \partial\mathbf{y}$ from observation space to gridpoint space, is not available as a stand-alone component of the regular NAVDAS code but it is currently being developed as part of the adjoint system.

Observation sensitivity can be used in a variety of ways to study the impact of observations on forecast outcome. For example, a Taylor series expansion can be used

to estimate the effect of an observation perturbation vector in terms of δJ

$$\delta J = \left\langle \delta \mathbf{y} \, , \, \frac{\partial J}{\partial \mathbf{y}} \right\rangle + \left\langle (\delta \mathbf{y})^2 \, , \frac{1}{2} \frac{\partial^2 J}{\partial \mathbf{y}^2} \right\rangle + \, ... \tag{11}$$

If the perturbations represented by $\delta \mathbf{y}$ do not exceed the magnitude of typical innovations, the Taylor series can be truncated to just the 1^{st}-order term

$$\delta J = \left\langle \delta \mathbf{y} \, , \, \frac{\partial J}{\partial \mathbf{y}} \right\rangle \, . \tag{12}$$

The scalar quantity δJ can represent the forecast impact caused by changes to real observations, or even the addition of hypothetical observations. It will be shown in Section 4.2 that observation sensitivity can also be used to quantify the impact of innovations (observation - background) on short-range forecast error differences. In fact, it is valid to interpret $\partial J \; / \; \partial \mathbf{y}$ as a sensitivity to the innovation vector, and $\delta \mathbf{y}$ as a perturbation or component of the innovation vector. Following (10) the impact of background perturbations can be evaluated using the expression

$$\delta J = \left\langle \delta \mathbf{x}_b \, , \, \frac{\partial J}{\partial \mathbf{x}_a} \right\rangle \; - \left\langle \mathbf{H} \, \delta \mathbf{x}_b \, , \, \frac{\partial J}{\partial \mathbf{y}} \right\rangle \, , \tag{13}$$

where the first term on the RHS of (13) is evaluated in gridpoint-space and the second RHS term is in observation space.

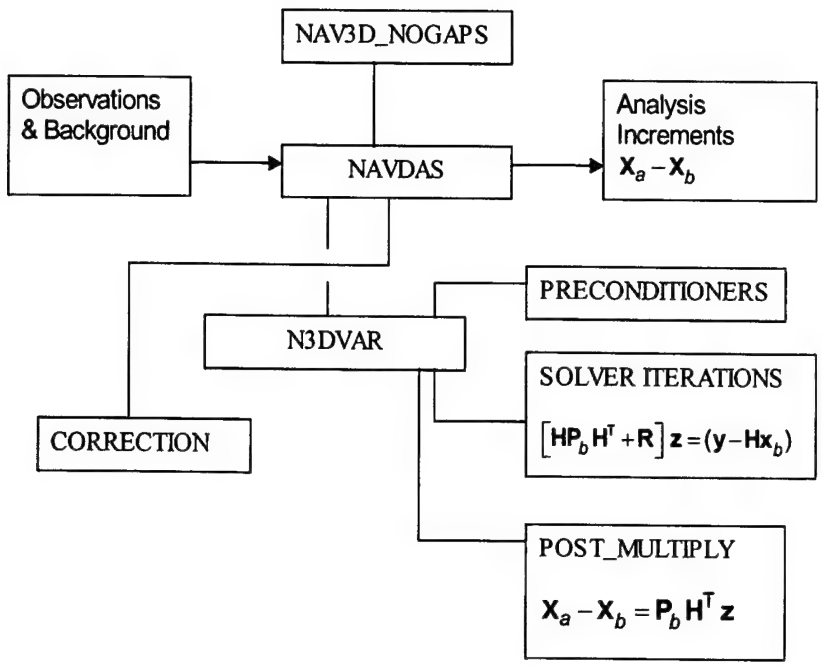

Figure 2: Primary subroutines in forward version of NAVDAS. Symbols are defined in Section 2.1.

2.2 Adjoint Code Description

The NAVDAS adjoint code is written in Fortran 90 and designed to run on multiple processors using MPI (message-passing-interface). The primary difference between the forward and adjoint codes for NAVDAS is the transposition of the post-multiplier.

Whereas in the forward NAVDAS (Fig. 2) the post-multiplier $\mathbf{P}_b\mathbf{H}^\mathbf{T}$ is applied after the solver $[\mathbf{HP}_b\mathbf{H}^\mathbf{T} + \mathbf{R}]^{-1}$, in the adjoint of NAVDAS (Fig. 3) the transpose of the post-multiplier $\mathbf{HP}_b$ is invoked first, and then the solver (which is the same in the forward and adjoint codes) is applied. In addition, the NAVDAS adjoint uses special routines for interpolation of the input analysis sensitivity vector $\partial J \ / \ \partial \mathbf{x}_a$ and for post–processing of the observation sensitivity output.

The computational time required to run the NAVDAS adjoint is less than that of the regular NAVDAS analysis, because the adjoint does not require that the innovation processing of the regular NAVDAS be repeated. The adjoint code is structured so that major functions are controlled by a driver program and several primary subroutines, which are described below. However, all details of the adjoint code development are not included here, and the actual Fortran code should be examined (see Appendix A) if additional information is required.

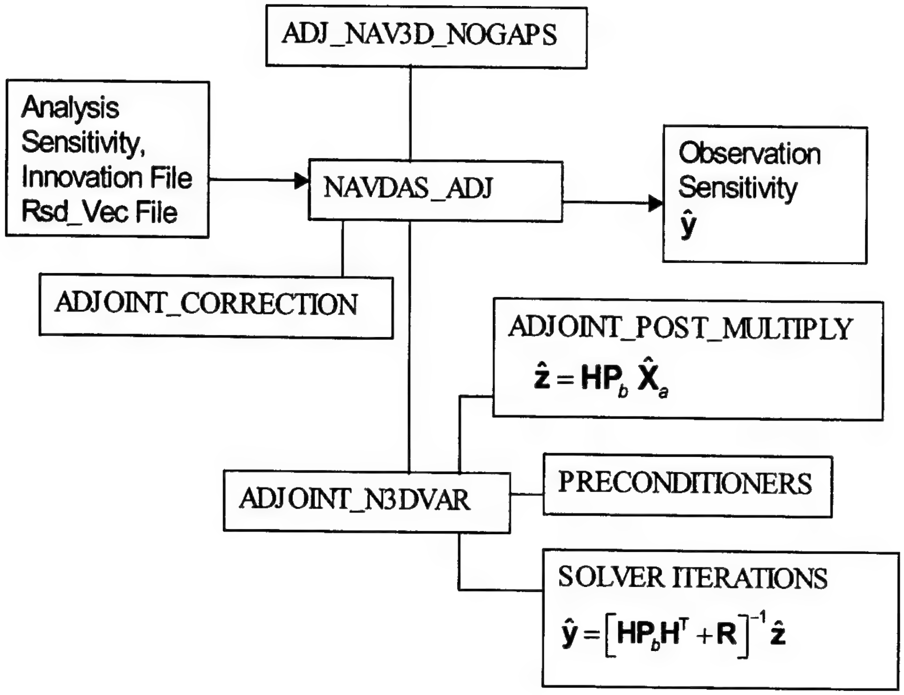

Figure 3: Primary subroutines in adjoint version of NAVDAS. Symbols are defined in Section 2.1. The caret (^) represents $\partial J/\partial(\ )$.

2.2.1 adj_nav3d_nogaps The main program module of the adjoint code is similar to the main program of the regular (forward) NAVDAS code (**nav3d_nogaps**), except that a call is made to **navdas_adj**, rather than to **navdas**. Certain parameters and switches are set differently for running the adjoint code. For example, the adjoint does not repeat any of the quality control checks that are performed in

the regular NAVDAS run. The quality control flag that results from the innovation and buddy check quality control is read from the **rsd_vec file** that has been produced in the regular NAVDAS run. The adjoint also reads a quality control flag from the **innovation file** that results from quality control checks in the NAVDAS pre-processor.

Switch Settings in NAVDAS Adjoint:

- innov_check = F
- buddy_check =F
- ghost = F (this is an option for ensuring that preconditioner prisms have sufficient observations in the regular NAVDAS)
- isentropic = F (the adjoint does not currently allow this option)
- jmin = F (the jmin diagnostics are not computed in the adjoint)
- analysis_error_exe = F (the call to **navdas_aerr** for analysis error estimates is not part of the adjoint code)

2.2.2 navdas_adj This subroutine reads the various input files required to run the NAVDAS adjoint, calls the major subroutines involved in the sensitivity calculations and writes the observation sensitivity to an output file. The first step is to read

the **innovation file** and **rsd_vec file** produced by the regular NAVDAS assimilation. These files contain information that specifies observation value, location, time, background value, errors assigned to the observation and background, quality control flags and other information valid at the assimilation time for which the sensitivity is to be calculated. The observations considered by the adjoint can be real observations provided in the **innovation file**, or they can be hypothetical observations defined by the user.

Subroutine	**Array(s)**	**Remarks**
navdas_adj	tempsen, usen, vsen	Analysis sensitivity (temperature, u-wind, v-wind) on the 1°, 60-level "output" grid of NAVDAS.
adjoint_correction	adjoint_eigen_grid	Analysis sensitivity in vertically-decomposed eigenvector space (60 levels).
adjoint_n3dvar	eob_work	Observation sensitivity in eigenvector space after call to adjoint_post_multiply
	cob	Observation sensitivity in physical space before call to solver
navdas_adj	ob_sens	Observation sensitivity vector in observation space after call to adjoint_n3dvar.

Table 1: Arrays that contain analysis and observation sensitivity in the NAVDAS adjoint code.

The analysis sensitivity vector $\partial J \,/\, \partial \mathbf{x}_a$ provided by the NOGAPS adjoint is read from a saved file and put into the arrays *tempsen*, *usen* and *vsen*, which contain the sensitivities for temperature, u-wind, and v-wind, respectively. The NOGAPS

adjoint also produces a sensitivity to terrain pressure, but this component is not used as input for the NAVDAS adjoint, because the forward NAVDAS does not produce a pressure analysis increment as an output field. An array *phisen* appears in the code but would be used only if the NOGAPS adjoint produced sensitivity to height instead of temperature. Note that a special interpolation procedure (see Section 3.1) is used to interpolate $\partial J \,/\, \partial \mathbf{x}_a$ from the NOGAPS grid to the NAVDAS grid before running the NAVDAS adjoint.

A call to **adjoint_correction** converts the sensitivity from the analysis gridpoint space to eigenvector space, and the sensitivity is then contained in the array *adjoint_eigen_grid* (Table 1). The subroutine **windrotate_grid** adjusts the analysis sensitivity winds from grid orientation to spherical coordinates, and **adjoint_n3dvar** is then called to perform the major part of the observation sensitivity calculations. Finally, **windrotate_ob** is called to convert the sensitivity winds (now in observation space) back to grid orientation from spherical coordinates. The observation sensitivity is then written to an output file.

2.2.3 adjoint_correction This subroutine is called from **navdas_adj** and converts the analysis sensitivity vector (contained in the arrays *tempsen, usen, vsen*) from NAVDAS gridpoint space to eigenvector space (*adjoint_eigen_grid*) near the beginning of the observation sensitivity calculations. The "zero-order" vertical interpolation option of NAVDAS is used here, because the 60 pressure levels used for

the arrays *tempsen*, *usen*, *vsen* have been specified to exactly match the 60 levels of *adjoint_eigen_grid*. The pressure levels for temperature and wind are defined by the arrays *prestout* and *pressout*, respectively. Also in this subroutine the temperature and wind sensitivities are "normalized" by multiplying with the square root of the background error variance (the array *rmsvar*).

2.2.4 adjoint_n3dvar This subroutine controls the two major components of the observation sensitivity calculations, which are the adjoint (transpose) of the NAVDAS post-multiplication step and the iterative application of the solver. At the beginning of this subroutine, the sensitivity is contained in the array *adjoint_eigen_grid* on the NAVDAS one-degree grid and in vertical eigenvector space using 60 vertical levels. The first major step is to apply the operator $\mathbf{HP}_b$ (the transpose of the forward NAVDAS post-multiplier $\mathbf{P}_b\mathbf{H}^\mathbf{T}$) to the analysis sensitivity as a "pre-multiplier" by calling the subroutine **adjoint_post_multiply**. The call to **adjoint_post_multiply** is actually made within a set of do-loops indexed over the number of analysis grid volumes and observation prisms.

After calling **adjoint_post_multiply** the sensitivity is contained in the array *eob_work* (Table 1). The subroutine **left_operator** converts the sensitivity from the eigenvector space of *eob_work* into the array *cob*, which is the sensitivity in physical (observation) space. The first and second preconditioners are applied and subroutine **genince** is then called to perform the iterative conjugate gradient solver

component of the NAVDAS adjoint, represented by $[\mathbf{HP}_b\mathbf{H}^\mathbf{T} + \mathbf{R}]^{-1}$. The solver subroutine (**genince**) is the same[2] in the forward and adjoint versions of NAVDAS, but the argument list in the call to **genince** is altered, as follows:

- call genince (w, xiv_ob, cob, ...)   in forward NAVDAS
- call genince (w, cob, ob_sens, ...)   in adjoint NAVDAS

In the forward NAVDAS, the solver input is the array *xiv_ob* and it returns the array *cob*, which is in observation space prior to the application of **right_operator**. In the adjoint NAVDAS, the solver input is the array *cob* and it returns the array *ob_sens*, which is the observation sensitivity in observation space. The final step in **adjoint_n3dvar** is a "de-normalization" of the sensitivity, accomplished by dividing *ob_sens* by the array *rmsvar*. The array *ob_sens* is then returned to **navdas_adj** for output.

2.2.5 adjoint_post_multiply This subroutine is called from **adjoint_n3dvar** and is used to apply the $\mathbf{HP}_b$ operator to the sensitivity vector in the first step of the NAVDAS adjoint calculations. It works in eigenvector space and represents the transpose of the operator $\mathbf{P}_b\mathbf{H}^\mathbf{T}$ performed by subroutine **post_multiply** in the forward NAVDAS. In the forward NAVDAS, the input for **post_multiply** is the

[2]The convergence criteria used in the descent algorithm of the solver are identical in the regular NAVDAS and adjoint NAVDAS.

array *eob_work* (the array *cob* projected into vertical eigenvector space) and the output is an array containing what is essentially the analysis correction vector in eigenvector space. In the adjoint NAVDAS, the input for **adjoint_post_multiply** is the sensitivity array *adjoint_eigen_grid* and the output is the adjoint version of the array *eob_work*.

2.2.6 Arrays used in NAVDAS adjoint

- *tempsen, usen, vsen* - sensitivity to temperature and winds (components of $\partial J \ / \ \partial \mathbf{x}_a$) on the 1° (lat-lon) 60-level NAVDAS output grid
- *adjoint_eigen_grid* - sensitivity to temperature and winds ($\partial J \ / \ \partial \mathbf{x}_a$) on the 1° (lat-lon) grid decomposed in vertical eigenvector space (60 levels)
- *ob_sens* - sensitivity to observations ($\partial J \ / \ \partial \mathbf{y}$) in observation space, currently includes temperature, wind, height, and brightness temperature observations
- *oberr_sens* - sensitivity to specified observation error in observation space, see Section 4.5 for definition
- *bkerr_sens* - sensitivity to specified background error in gridpoint space, currently not implemented
- *prestout, pressout* - defines the 60 pressure levels used for input of temperature and wind analysis sensitivity, respectively

- *xiv_ob* - innovation values read from the **innovation file** produced by NAVDAS
- *rsd_val* - residual (analysis - observation) values read from the **rsd_vec file** produced by NAVDAS
- *num_reject* - observation reject flag values read from the **rsd_vec file** produced by NAVDAS
- *cob_fwd* - "cob" vector from the regular (forward) NAVDAS read from the **rsd_vec file**

3 Running the NAVDAS Adjoint

The NAVDAS adjoint code exists as a single file written in Fortran 90 called **NAVDAS_adj.f** that contains the main program and all required subroutines and defined functions. The source code is compiled using a **makefile** that produces the executable **NAVDAS_adj.exe**. There is no attached code library. The adjoint calculation uses an outer c-shell script called **run_navdas_adjoint**. The c-shell script controls input and output of certain files used by the adjoint and invokes a k-shell script called **NAVDAS_adj.ksh** that invokes the NAVDAS adjoint executable file. The NAVDAS adjoint source code and scripts are available in a directory on the NRL computer **hadley** (see Appendix A). The procedure for calculating observation sensitivity with the NAVDAS adjoint includes the following steps:

Procedure for Calculating Observation Sensitivity:

1. Run the regular NAVDAS assimilation to produce analyzed initial conditions. Save the **innovation file** and **rsd_vec file**

2. Run the full-physics nonlinear forecast model (NOGAPS) and save the forecast trajectory

3. Define a forecast costfunction (J)

4. Run the NOGAPS adjoint to produce the analysis (initial condition) sensitivity $\partial J \ / \ \partial \mathbf{x}_a$

5. Interpolate $\partial J \ / \ \partial \mathbf{x}_a$ from the NOGAPS gaussian grid to the NAVDAS output grid (see Section 3.1, below)

6. Run the NAVDAS adjoint to produce the observation sensitivity $\partial J \ / \ \partial \mathbf{y}$

7. Run graphics or post-processing to plot observation sensitivity, observation impact or other products

3.1 Pre-Processing (Interpolation of $\partial J \ / \ \partial x_a$)

The analysis sensitivity vector $\partial J \ / \ \partial \mathbf{x}_a$ comprises the "input" to the NAVDAS adjoint and is provided on a 1° lat-lon grid with 60 vertical levels that correspond exactly to the levels used in the vertical eigenvector decomposition at the end of the regular NAVDAS analysis. This allows the zero-order interpolation option to be used when the arrays that contain $\partial J \ / \ \partial \mathbf{x}_a$ (*tempsen*, *usen*, *vsen*) are transferred into

adjoint_eigen_grid by the subroutine **adjoint_correction**.

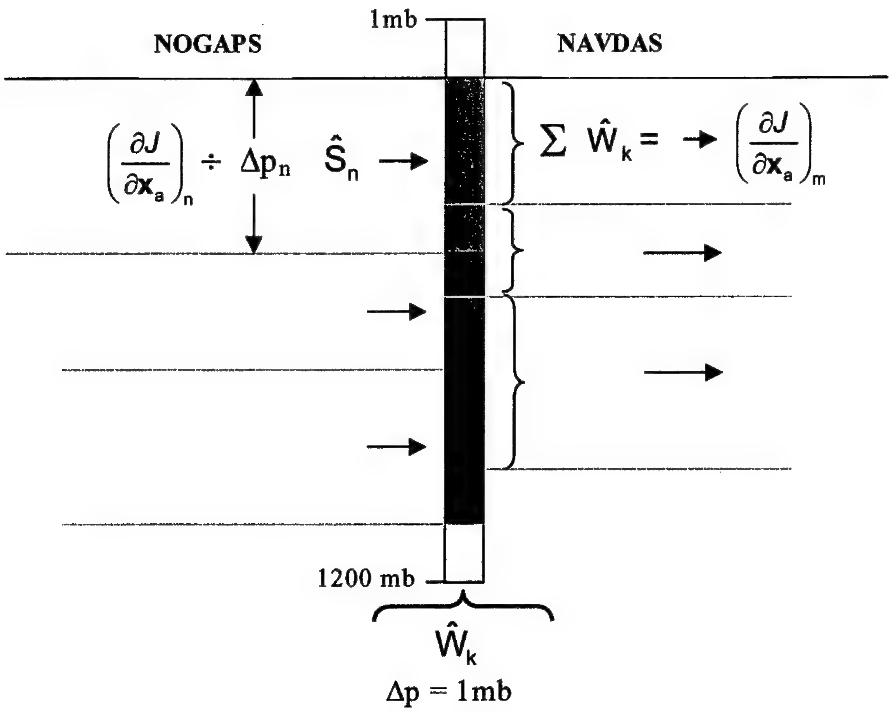

Figure 4: Interpolation of an adjoint sensitivity gradient between grids with different vertical configurations. Used for transfer of analysis sensitivity from NOGAPS sigma levels to NAVDAS output pressure levels in the pre-processing step for NAVDAS adjoint. $\hat{\mathbf{W}}$ is an array that contains the analysis sensitivity values normalized to represent pressure intervals of 1 mb.

Before running the NAVDAS adjoint, a special pre-processing interpolation procedure is required to transfer $\partial J / \partial \mathrm{x}_a$ from the NOGAPS gaussian grid and sigma surfaces onto the NAVDAS grid. Because the adjoint sensitivity fields are gradients,

rather than conventional temperature or wind variables, this interpolation step must carefully account for differences in horizontal and vertical resolution of the NOGAPS and NAVDAS grids. It is critical that this step be performed correctly, so that the global sum of the analysis sensitivity is identical on both grids. Other procedures, such as bi-linear interpolation, should not be used to interpolate adjoint sensitivity between grids with different horizontal or vertical resolutions, as they are likely to introduce serious distortion of the sensitivity gradients. A version of the pre-processing sensitivity interpolation procedure for NAVDAS is provided as a Fortran 90 file called **gradtp.f** (see Appendix A).

The first step in the interpolation of the analysis sensitivity (temperature and winds) is a transfer of $\partial J \;/\; \partial \mathbf{x}_a$ from NOGAPS sigma-levels to the 60 constant-pressure levels used by NAVDAS, at every point on the NOGAPS gaussian grid. The procedure is illustrated in Fig. 4.

1. The sensitivity ($\partial J \;/\; \partial \mathbf{x}_a$) values on each NOGAPS sigma level are normalized by the thickness of the pressure layer (in mb) that each level represents. Thus, for some level, n with a pressure thickness $(\Delta p)_n$, we let $\hat{S}_n = (\partial J \;/\; \partial \mathbf{x}_a)_n \;/\; (\Delta p)_n$.

2. The values of of $\hat{S}_n$, for all n levels of NOGAPS, are used to define the elements of an array, $\hat{W}$, that contains the normalized sensitivity values at 1 mb vertical intervals from 1 mb to 1200 mb. Thus, if sigma level n represents pressure from 500 - 600 mb at a NOGAPS gridpoint, the value $\hat{S}_n$ is assigned to each of the

k elements of $\hat{W}$ from k=500 to 600 mb. Any elements of $\hat{W}$ below the NOGAPS surface terrain pressure are assigned a value of zero.

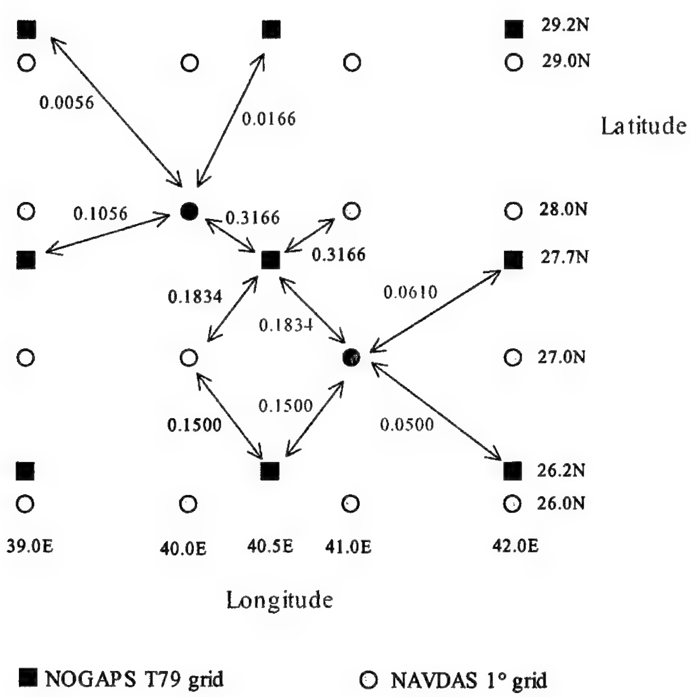

Figure 5: Example of interpolations performed on constant pressure surfaces between the NAVDAS 1° grid and the NOGAPS T79 grid (shown with a resolution of exactly 1.5° here to simplify the diagram). The weighting factors on arrows directed towards NOGAPS points represent interpolation of conventional fields and add to 1.0. The weighting factors on arrows directed towards NAVDAS points represent interpolation of sensitivity gradient fields and add to 0.4444, which is the ratio of the areas represented by grid points on the 1° grid and the 1.5° grid, 0.4444 = ((1.0*1.0) ÷ (1.5*1.5)). NAVDAS 1° gridpoints represent smaller areas than NOGAPS T79 gridpoints, and the sensitivity magnitude is reduced through this interpolation to account for the difference. Interpolation weighting factors are determined by procedures illustrated in Figs. 6 and 7. In practice, all grid points are used in the interpolations.

3. The normalized sensitivity is then transferred from the array $\hat{W}$ onto the 60-level NAVDAS grid, in the reverse sense of Steps 1 and 2. Each of the 60 levels on the NAVDAS grid represents a layer pressure thickness. Thus, if pressure level m represents pressure from 520 - 560 mb on the NAVDAS grid, the value $(\partial J \ / \ \partial \mathbf{x}_a)_m$ is the sum of the k elements of $\hat{W}$ from k=520 to 560. Note that the pressure levels for temperature are not the same as for wind.

4. After completion of this step, the values of $\partial J \ / \ \partial \mathbf{x}_a$ in any vertical column can be summed over all sigma levels on the NOGAPS grid and over all pressure levels on the NAVDAS grid and the two sums should be identical.

The second interpolation step is a transfer of $\partial J \ / \ \partial \mathbf{x}_a$ from the gaussian grid of NOGAPS to the 1° lat-lon NAVDAS grid, on each of the 60 levels defined in the previous step. This horizontal interpolation is designed to conserve the global sum of the sensitivity gradient when it is transferred between grids with different resolutions. The "forward" interpolation is a transfer of conventional fields (temperature, wind) from the NAVDAS grid to the NOGAPS grid. As shown in Fig. 5, the weighting factors on arrows directed from NAVDAS to NOGAPS points (in the forward interpolation sense) add to 1.0, which conserves the values of the conventional variables. In contrast, the weighting factors on arrows directed from NOGAPS to NAVDAS points (in the adjoint interpolation sense) add to 0.4444, which is the ratio of the areas represented by grid points on the NAVDAS 1° grid vs. the NOGAPS T79 grid

(~1.5°). Thus, the sensitivity magnitude at individual grid points on the 1° grid is less than on the T79 grid, because each 1° gridpoint represents a smaller area, but the global sum of the sensitivity over all points on each grid is identical. Different weighting factors would be used when the resolution of either the NOGAPS gaussian grid or the NAVDAS grid is changed.

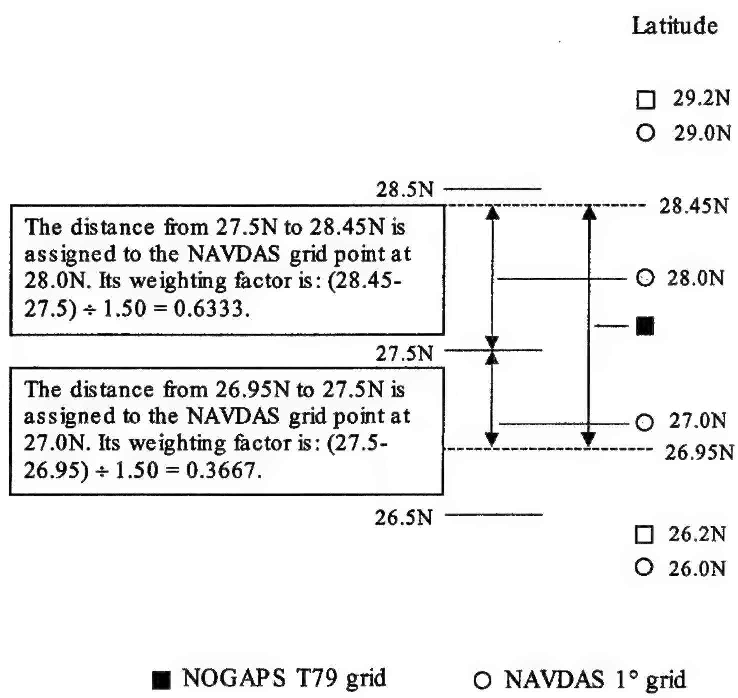

Figure 6: Example of interpolation weighting factors based on north-south distance. In this example, the interpolation is from NAVDAS grid points to the NOGAPS grid point at 27.7N, which represents a distance of 1.5° from 26.95N to 28.45N. The total weighting factor depends also on the east-west grid configuration (Fig. 7).

Weighting factors for horizontal interpolation (like those shown in Fig. 5) are determined by a linear algorithm based on distances in the north-south and east-west directions. Consider the "forward" interpolation from the NAVDAS grid to the NOGAPS grid. Each T79 grid point represents a north-south distance of 1.5° (approximately 1.5° on the actual T79 grid), centered on the gridpoint latitude. If the latitude of the T79 gridpoint is, say, 27.7N, it represents the interval from 26.95N to 28.45N, as shown in Fig. 6. This interval on the T79 grid is overlapped by intervals represented by several (either two or three) points on the NAVDAS 1° grid. In the example of Fig. 6 the interpolation to the T79 grid point at 27.7N is a weighted average of values taken from points on the NAVDAS 1° grid at 27N and 28N. The total weighting factor for horizontal interpolation is a product of the north-south weighting factor and another factor that depends on the east-west grid configuration, as shown in Fig. 7. If the longitude of the T79 gridpoint is an integer (e.g., it lies directly on the 1° grid at gridpoint "i") the assigned weighting is 1/6 to the column indexed (i-1), 2/3 to the column indexed (i) and 1/6 to the column indexed (i+1). In the alternate case where the T79 gridpoint is halfway between points on the 1° grid, the two columns to the east and west are each assigned half the weight.

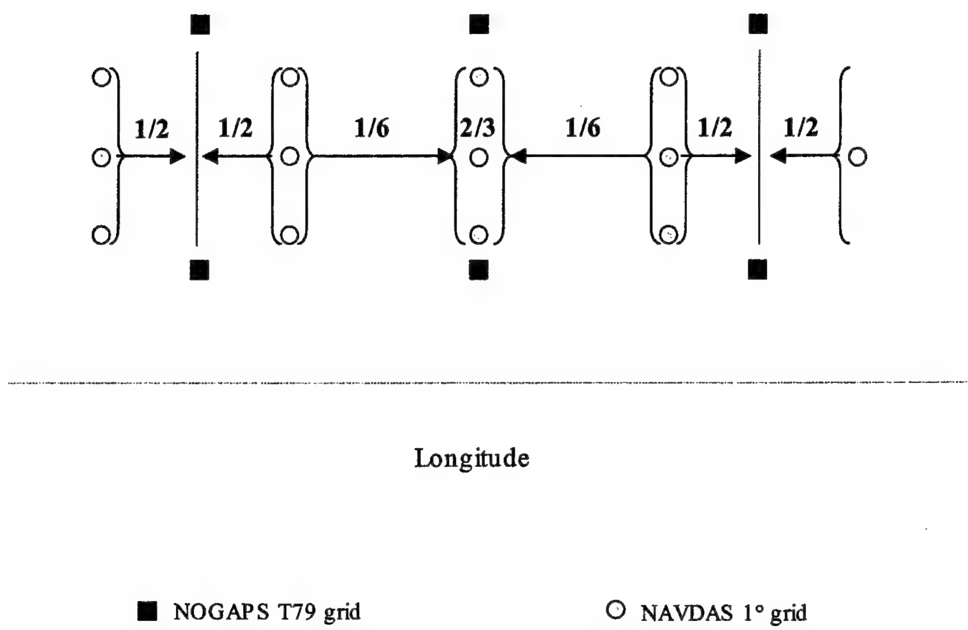

Figure 7: Interpolation weighting based on longitudinal position of NAVDAS and NOGAPS gridpoints. The total horizontal interpolation weighting factor as shown for selected gridpoints in Fig. 5 combines a weighting factor for the east-west direction (illustrated here) and a weighting factor for the north-south direction as illustrated in Fig. 6.

3.2 Output File

The output of the NAVDAS adjoint is written to a formatted file. Each line of the output file corresponds to a separate observation (excluding any rejected observations), and includes the following information:

- n - sequence number of observation
- rlat_ob - latitude of observation
- rlon_ob - longitude of observation
- ob_sens - observation sensitivity, $\partial J \ / \ \partial \mathbf{y}$
- adjoint cob - $(\ \widehat{\mathbf{z}} = \mathbf{H}\,\mathbf{P}_b\ \partial J \ / \ \partial \mathbf{x}_a)$
- jvarty_ob - observation type (1=height, 2=temperature, 3=u-wind, 4=v-wind, 13=brightness temperature)
- insty_ob - instrument type
- num_reject - reject flag (0=assimilated, 1=rejected)
- err_ob - assigned observation error standard deviation
- rmsvar - assigned background error standard deviation
- p_ob - pressure level of observation
- c_pf_ob - observation label (pt. 1)
- c_db_ob - observation label (pt. 2)
- xiv_ob - innovation (observation - background)
- ob - observation value

- oberr_sens - sensitivity to observation error standard deviation

- rsd_val - residual (analysis - observation)

3.3 Gradient (accuracy) Test

A basic procedure for validating that an adjoint model has been correctly coded is the so-called gradient test, which compares the value of scalar inner products, using input and output sensitivity vectors. With the NAVDAS adjoint, a form of the gradient test can be defined as

$$\underbrace{\left\langle (\mathbf{y} - \mathbf{H}\mathbf{x}_b) \, , \, \frac{\partial J_f^g}{\partial \mathbf{y}} \right\rangle}_{\substack{observation-space \\ \delta J_{obs}}} = \underbrace{\left\langle (\mathbf{x}_a - \mathbf{x}_b) \, , \, \frac{\partial J_f}{\partial \mathbf{x}_a} + \frac{\partial J_g}{\partial \mathbf{x}_b} \right\rangle}_{\substack{gridpoint-space \\ \delta J_{grid}}} \, , \tag{14}$$

where the LHS of (14) is calculated in observation space using temperature, wind, and height innovations and sensitivity, and the RHS is calculated in the gridpoint space of the forecast model using temperature, wind, and terrain pressure analysis increments and sensitivity. For consistency with results shown later, it is convenient to define the costfunction here so that δJ represents the *difference* between the forecast errors of trajectories starting from $\mathbf{x}_a$ and $\mathbf{x}_b$. Thus, e_f is the error in a forecast of length f starting from $\mathbf{x}_a$,and e_g is the error in a forecast of length g starting from $\mathbf{x}_b$. The 6-hr forecast of trajectory g provides the background for the assimilation that produces

$\mathbf{x}_a$, and the two forecasts verify at the same time. The scalar quantities δJ_{obs} and δJ_{grid} are adjoint-based estimates of the actual error difference $e_f - e_g$. Appendix B provides a derivation of the expressions used in (14). Note that the forecast length does not affect the accuracy of this gradient test, since the test only depends on the accuracy of the NAVDAS adjoint calculation (e.g., Eq. 1) and not on the accuracy of the forecast model (NOGAPS) adjoint. However, forecast length *does* affect the accuracy of δJ_{obs} and δJ_{grid} *with respect to the actual value of* $e_f - e_g$ that is obtained from the nonlinear forecast model (see Section 4.2).

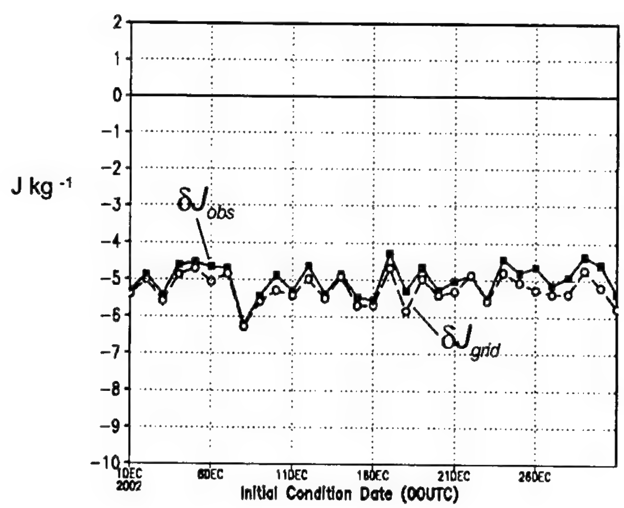

Figure 8: Gradient test comparison for δJ_{obs} (solid line) and δJ_{grid} (dash line) for Dec 2002. Costfunction J is NOGAPS forecast error (e_{24}-e_{30} , J kg^{-1}) in the global domain. δJ_{obs} and δJ_{grid} are defined in Section 3.3.

A comparison of δJ_{obs} with δJ_{grid} using $f = 24h$ and $g = 30h$ for the month of December 2002 is shown in Fig. 8. The forecast errors are calculated in the global domain from NOGAPS forecasts started at 00UTC. For December 2002, the average value of $\delta J_{obs}/\delta J_{grid}$ is 0.951 (maximum = 1.002, minimum = 0.883). These results indicate that the NAVDAS adjoint calculates the observation sensitivity from the analysis sensitivity input to within about 95% accuracy. Note that δJ is negative, since $e_{24} < e_{30}$.

In theory the equivalence of δJ_{obs} and δJ_{grid} should be exact if the adjoint code that produces the sensitivity $\partial J \ / \ \partial \mathbf{y}$ is completely consistent with respect to the version of NAVDAS that produces the analysis increment $(\mathbf{x}_a - \mathbf{x}_b)$ from the innovation $(\mathbf{y} - \mathbf{H}\mathbf{x}_b)$. In practice, there are several obstacles that prevent an exact result. First, the interpolation of $\partial J \ / \ \partial \mathbf{x}_a$ from NOGAPS to NAVDAS gridpoint space unavoidably introduces some small (but finite) inaccuracy into the observation sensitivity results.

An additional consideration is that the NOGAPS adjoint produces a sensitivity to the analyzed terrain pressure as a component of $\partial J \ / \ \partial \mathbf{x}_a$, but this pressure sensitivity does not directly translate into a component of the sensitivity input to NAVDAS, because NAVDAS does not produce a pressure analysis increment. Since the terrain pressure contribution to the input analysis sensitivity from NOGAPS is neglected in Fig. 8, there is a small systematic underestimate of the observation sensitivity magnitude in the NAVDAS adjoint calculation.

3.4 Code Maintenance and Updating

The current version of the NAVDAS adjoint is consistent with the forward version of NAVDAS as of January 2004. It is anticipated that the adjoint code will be updated at periodic intervals in order to maintain applicability to the operational data assimilation system. For example, new observation quantities such as ozone will be added to the adjoint code. However, the NAVDAS adjoint should be considered a research code and it is not part of the formal NAVDAS configuration management system. Refer to Appendix A for the locations of current codes and scripts.

4 Observation Sensitivity Examples

The current version of the NAVDAS adjoint provides two sensitivity gradients, i) the sensitivity to observations $\partial J \,/\, \partial \mathrm{y}$ and ii) the sensitivity to the assigned observation error (see Section 4.5). The observation sensitivity $\partial J \,/\, \partial \mathrm{y}$ can be used for a variety of applications, which involve various choices of observation (or innovation) perturbation δy and costfunction J. Four possible applications are summarized in Table 2. Application #1 is the use of observation sensitivity to interpret arbitrary perturbations of the observations or background. In application #2, we quantify the impact of actual innovations on a known forecast error difference. Application #3 describes the general interpretation of sensitivity for hypothetical observations. Application #4 pertains to targeted observing, when the both innovations and forecast errors are

not known.

Application	δy	***J* (scalar)**
1. Basic Observation Sensitivity: What are the impacts of various observation perturbations ?	Any perturbation of appropriate size	Any valid costfunction
2. Innovation Impact: What are the impacts of actual innovations on a known forecast error ?	$\mathbf{y} - \mathbf{Hx}_b$ (all known)	Forecast error (known)
3. Hypothetical Observations: What are the impacts of hypothetical observations on a known forecast error ?	$\mathbf{y} - \mathbf{Hx}_b$ (some known, some unknown)	Forecast error or other costfunction
4. Targeted Observing: What is the impact of adding a set of targeted observations to the regular observing network at a future time?	$\mathbf{y} - \mathbf{Hx}_b$ (all unknown)	Costfunction usually a forecast error surrogate

Table 2: Examples of observation sensitivity applications.

4.1 Basic Observation Sensitivity

In the most general application, observation sensitivity can be used to estimate the effect of various arbitrary changes in the values of observations (or innovations). For example, we can define J as the difference between the 24h and 30h global forecast error and examine the sensitivity of this costfunction with respect to any component of the observation vector, as illustrated in Fig. 9 for rawinsonde temperature observations assimilated at 00UTC 10 December 2002. The sensitivity vector $\partial J \ / \ \partial \mathbf{y}$ is plotted in observation space at the locations where observations have been assimilated by NAVDAS. We can also define an observation perturbation vector $\delta \mathbf{y}$, which can represent a change to the value of any one, or all, observations assimilated by NAVDAS. Using (12), the perturbation $\delta \mathbf{y}$ implies that the forecast costfunction will be changed by an amount δJ. Thus, if we consider one temperature observation for which (suppose) $\partial J \ / \ \partial \mathbf{y}$ = 0.004 J kg^{-1}deg^{-1}, and we let $\delta \mathbf{y}$ = 2.0 deg, then δJ = 0.008 J kg^{-1}. The magnitude of $\delta \mathbf{y}$ is normally restricted to perturbations no larger than typical innovations because of tangent linear approximations in the forecast model adjoint, and the sensitivity information is most accurate for short-range forecasts of 72h or less.

In addition to estimation of observation perturbation impact, the observation sensitivity $\partial J \ / \ \partial \mathbf{y}$ and the analysis sensitivity $\partial J \ / \ \partial \mathbf{x}_a$ can be used to determine the value of δJ implied by a background perturbation $\delta \mathbf{x}_b$, using (13), as described

in Section 2.2.

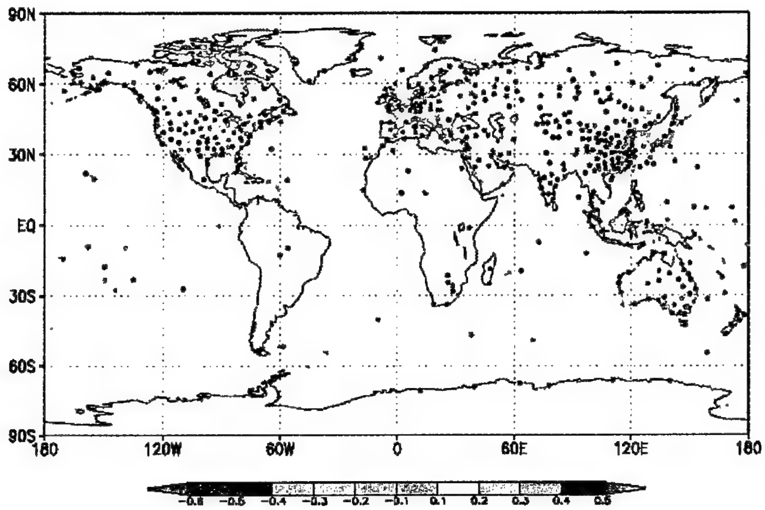

Figure 9: Sensitivity of $J = \mathbf{e}_{24}\text{-}\mathbf{e}_{30}$ to 500 mb rawinsonde temperature observations at 00UTC 10 Dec 2002. Units are 10^{-3} J kg^{-1}deg^{-1}.

4.2 Observation Impact On Forecast Error

Observation sensitivity can be used in a diagnostic mode to evaluate the impact of actual observations (or innovations) on the difference between two short-range forecast errors. As in Section 3.3, we define e_f as the error in a forecast of length f starting from $\mathbf{x}_a$, and e_g is the error in a forecast of length g starting from $\mathbf{x}_b$. The 6-hr forecast of trajectory g provides the background for the assimilation that

produces $\mathbf{x}_a$, and the two forecasts verify at the same time. In general, $\mathbf{x}_a$ will be a better estimate of the true atmospheric state than $\mathbf{x}_b$, and thus typically (but not always) $e_{24} < e_{30}$. The error difference $e_f - e_g$ is due entirely to the assimilation of observations used to produce the analysis $\mathbf{x}_a$. The true difference between the forecast errors e_f and e_g is

$$\Delta e_f^g = e_f - e_g \ . \tag{15}$$

Note that in a limiting case in which no observations are assimilated, $\mathbf{x}_a = \mathbf{x}_b$ and $\Delta e_f^g = 0$. As shown in Langland and Baker (2004) and in Appendix B, observation sensitivity can be used to provide an estimate of Δe_f^g, using what can be called an "observation impact" equation

$$\delta e_f^g = \left\langle (\mathbf{y} - \mathbf{H}\mathbf{x}_b) \ , \ \frac{\partial J_f^g}{\partial \mathbf{y}} \right\rangle \ . \tag{16}$$

For the global domain, the inner product represented by (16) is evaluated using the entire innovation and observation sensitivity vectors (excluding moisture at present). Note that for this choice of costfunction δe_f^g in (16) is the same quantity as δJ_{obs} in (14). It can also be noted that studies by Doerenbecher and Bergot (2001) and Fourrie et al. (2002) use observation impact functions in observation space that are similar in form to Eq. (16) - e.g., they involve the innovation vector and an observation sensitivity gradient However, in those studies the observation sensitivity is not derived with an actual adjoint of the assimilation procedure. Fourrie et al. (2002) use the error difference $e_f - e_g$ as a costfunction, but their impact function is

based on sensitivity gradients that involve only the trajectory starting from $\mathbf{x}_a$. In Doerenbecher and Bergot (2001), the costfunction is a dynamic variable (enstrophy), rather than a forecast error.

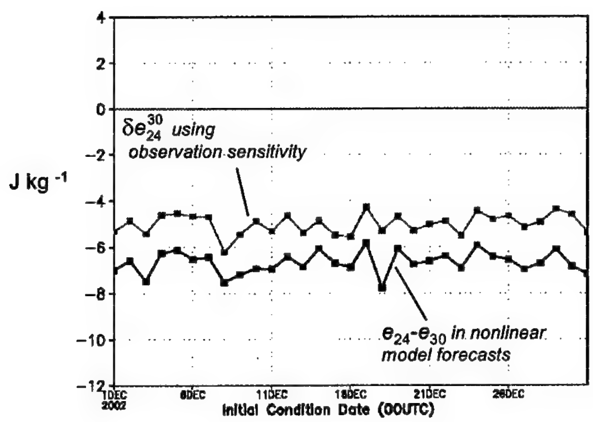

Figure 10: Time series of $\mathbf{e}_{24}$-$\mathbf{e}_{30}$ (dark solid line) in NOGAPS forecasts and corresponding adjoint-based observation impact estimate δe_{24}^{30} (grey solid line) calculated using Eq. 16 in the global domain with no moisture observations in December 2002.

A time series comparing Δe_f^g and δe_f^g for December 2002, using $f = 24h$ and $g = 30h$ is provided in Fig. 10. The values of δe_{24}^{30} and Δe_{24}^{30} are negative, since $e_{24} < e_{30}$. For December 2002, the average value of δe_{24}^{30} / Δe_{24}^{30} is 0.740 (maximum = 0.827, minimum = 0.672). The observation impact calculations using (16) are thus an underestimate of the actual forecast error difference. The majority of the

underestimate is probably explained by the neglect of moisture observations[3] in the current NAVDAS adjoint. However, the accuracy of the observation impact estimate is also affected by approximations in the forecast model adjoint, primarily the neglect of moist physical processes and nonlinearities in the dry dynamics. The effect of these tangent linear approximations becomes more significant as forecast length increases.

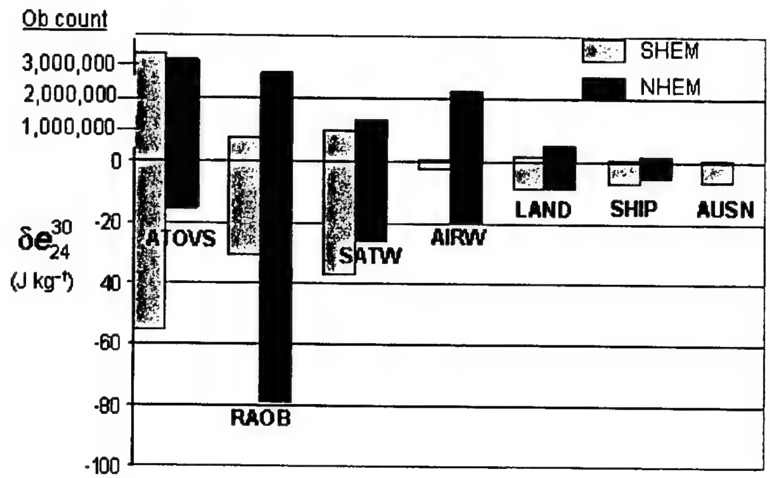

Figure 11: Summed global observation impact (δe_{24}^{30} , J kg^{-1}) for Southern and Northern Hemisphere, partitioned by instrument type, combining June and December 2002. Includes all observations assimilated in NAVDAS at 00UTC. ATOVS-temperature retrievals, RAOB-rawinsondes, SATW-cloud and feature-track winds, AIRW-commercial aircraft observations, LAND-land surface observations, SHIP-ship surface observations, AUSN-synthetic sea-level pressure data

[3]Moisture data account for about 30 percent of total global observations at 00UTC.

Fig. 11 illustrates how observation impact estimates can be used to compare the value provided by the various types of observations assimilated by NAVDAS. Here, observation impact is evaluated in terms of δe_{24}^{30} for the northern and southern hemispheres, combining the months of June and December 2002 and using observations assimilated at 00UTC. ATOVS are satellite temperature retrievals (Reale et al. 2003). SATW are feature-track wind vectors from visible, microwave and water vapor geostationary imagery (Rao et al. 2002). RAOB are rawinsonde temperature, winds, and surface heights. AIRW are commercial aircraft temperature and wind data in level flight and ascent and descent profiles. LAND are surface temperatures, winds, and heights from land surface reporting stations. SHIP are surface temperatures, winds, and heights from ships at-sea. AUSN are synthetic sea-level pressure data assimilated as height observations over part of the southern hemisphere (Guymer 1978).

As shown in Fig. 11, the largest forecast error reductions (δe_{24}^{30}) for the southern hemisphere from observations assimilated at 00UTC are produced by ATOVS, satellite wind data, and rawinsondes. In the northern hemisphere the largest error reductions are produced by rawinsonde, satellite wind data, commercial aircraft data and ATOVS. Almost all the error reduction due to commercial aircraft observations is attributable to data in the northern hemisphere. Land and ship surface data produce lesser (but still significant) forecast error reductions. AUSN data are a valuable observation type for the southern hemisphere. In fact, the error reduction *per obser-*

vation for AUSN can be much larger than for other types of observations (Langland and Baker 2004).

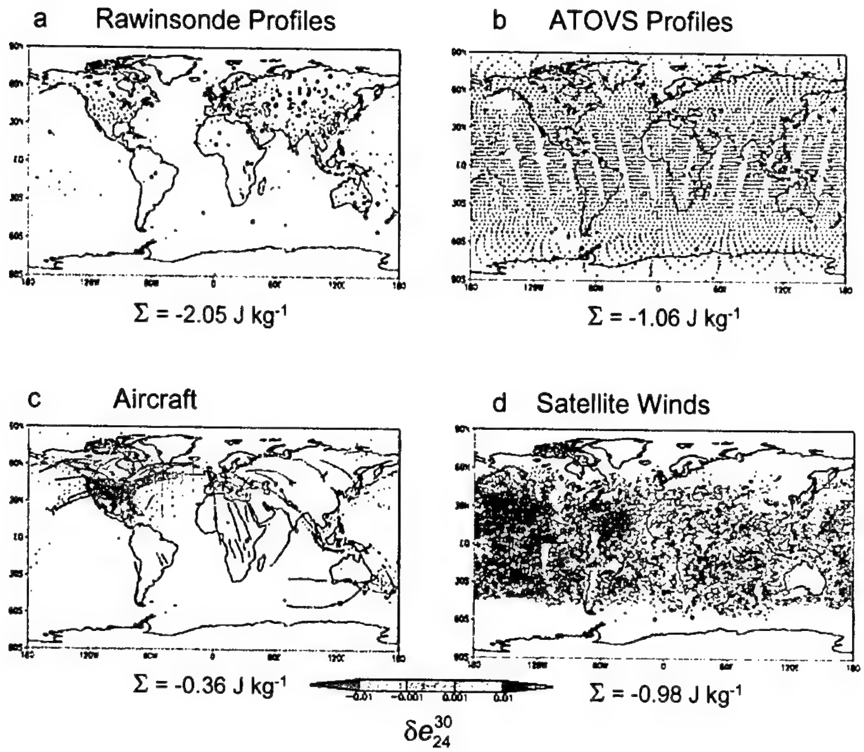

Figure 12: Observation impact (J kg^{-1}) in the NAVDAS assimilation at 00UTC 10 December 2002. Green (red) dots represent large reduction (increase) in 24h global forecast error. Blue (orange) dots represent moderate reduction (increase) in 24h global forecast error. Grey dots represent relatively small reduction or increase in 24h global forecast error. For rawinsondes and ATOVS each dot represents the combined impact of observations in vertical profiles. For aircraft and satellite wind observations each dot combines the impact of observations with the same latitude, longitude and pressure level. Σ = global sum of observation impact for instrument type.

While Fig. 11 indicates that the global (or hemispheric) sums of δe_{24}^{30} are negative (confirming that assimilation of large numbers of observations reduces $e_{24} - e_{30}$) these sums combine large numbers of positive, as well as negative, observation impacts associated with individual observations. This can be seen by examining the pattern of observation impact at a particular assimilation time. For example, at the assimilation time of 00UTC 10 Dec 2002 (Fig. 12), each of the four observation types include many individual data for which $\delta e_{24}^{30} > 0$ (shown as orange and red dots). This mix of positive and negative observation impact at a single assimilation time does not indicate a systematic problem with certain observations, rather it is an outcome of the statistical assumptions and approximations used in data assimilation. However, if the impact of a particular observation type or reporting station is *consistently* > 0, it could indicate an instrument or quality control problem.

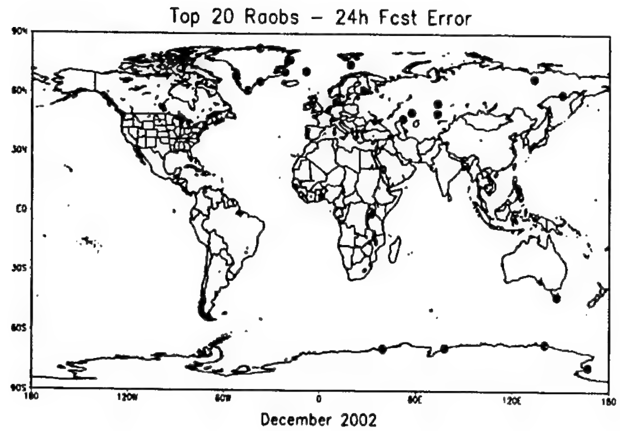

Figure 13: Twenty rawinsonde observing stations that produce the largest observation impact δe_{24}^{30}, representing reductions of e_{24}-e_{30} in the global domain, due to observations assimilated at 00UTC in December 2002.

Another example of observation impact (Fig. 13) shows the locations of 20 rawinsonde stations that produced the largest negative values (e.g., error reduction) of δe_{24}^{30} for 00UTC assimilations and forecasts during the month of December 2002. These "key" rawinsondes tend to be found along land / ocean boundaries, in regions where forecast error growth rates are relatively large, and where other in-situ or satellite observations are relatively sparse.

4.3 Hypothetical Observations

The NAVDAS adjoint can be used to determine the sensitivity of a known forecast error or forecast parameter to hypothetical, as well as "real" observations. The following information must be provided for each of the hypothetical observations:

- Latitude and Longitude
- Pressure Level
- Instrument Type (e.g., rawinsonde, satellite wind, etc.)
- Observation type (e.g., temperature, wind, height)
- Specified observation error

In this application the costfunction (J) can be forecast error or some other forecast parameter of interest, such as surface pressure, or wind speed. The NAVDAS adjoint will produce sensitivity to both the real and hypothetical observations. Note that the observation sensitivity can be determined without the specification of an innovation value. The impact of the real observations on an actual short-range forecast error difference can be calculated using (16). The impact of the hypothetical observations can also be estimated using (16), if a proxy innovation value is specified. Sensitivity to hypothetical observations can be used, for example, to develop more optimal configurations of satellite and in-situ observing systems.

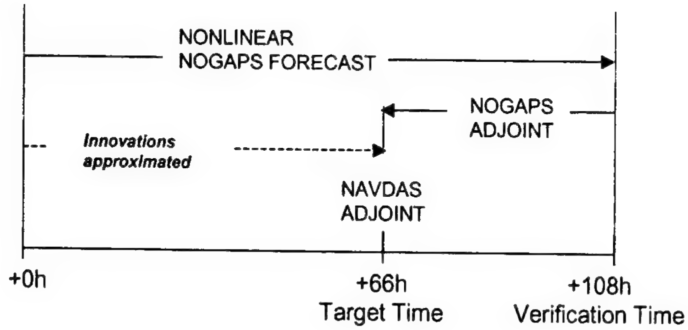

Figure 14: Configuration for targeted observing used in Fig. 15. The interval from +0h to +66h is used to produce the targeting guidance and deploy observational resources to the target area.

4.4 Targeted Observing

Observation sensitivity can be used for "targeted observing," in which objective (model-based) information provides guidance for the deployment of special observations intended to improve a short-range numerical weather forecast over a specific region. This is a variant of sensitivity to hypothetical observations, in which a costfunction other than actual forecast error must be used, and the observation sensitivity is calculated for a future time (typically 24-72h ahead) when the targeted observations are to be assimilated. An example of a possible time configuration for targeted observing is shown in Fig. 14. Usually, the "targeted observations" will be

a relatively small set of special data added to the observations provided by regular satellite and in-situ observing systems. The goal of targeted observing is to *maximize the value of the complete observing network*, e.g, the regular observations *plus the special targeted observations.* However, adding targeted observations will, in general, change the impact of nearby regular observations. The targeted observing procedure generally includes the following steps:

Procedure for Targeted Observing:

1. Identify the forecast feature that is to be improved, through examination of deterministic or ensemble forecasts

2. Define a forecast verification region, verification time and costfunction (J)

3. Define the type of targeted observation(s) and time at which they are to be obtained

4. Define several (or many) possible configurations for the targeted observations

5. Calculate observation sensitivity $\partial J \ / \ \partial \mathbf{y}$ for each configuration (each requires a separate run of NAVDAS adjoint)

6. Prioritize targeting configuration based on impact function (e.g., Eq. 18, Eq. 19, or other expression)

7. Obtain targeted observations using in-situ or satellite instruments

8. Assimilate targeted observations and produce forecast

In step 5, the locations of the hypothetical targeted observations can be specified using an input file read by the NAVDAS adjoint. The locations of regular rawinsonde, land-surface, and ATOVS observations at the future targeting time can be estimated with fairly good accuracy. The locations of commercial aircraft and feature-track satellite wind data can be approximated using information from the most-recent analysis performed at the same hour (e.g., 00UTC, 18UTC, etc.) as the time at which the targeted observations are to be taken. The costfunction J for targeted observing can be a forecast parameter, such as vorticity, wind, temperature, or surface pressure, or it can be a difference between two forecasts, but the costfunction in targeted observing cannot be forecast error, since that is not known in advance. Another constraint is that the actual innovation values are not known for any of the observations, either real or hypothetical, that will be obtained at the targeting time.

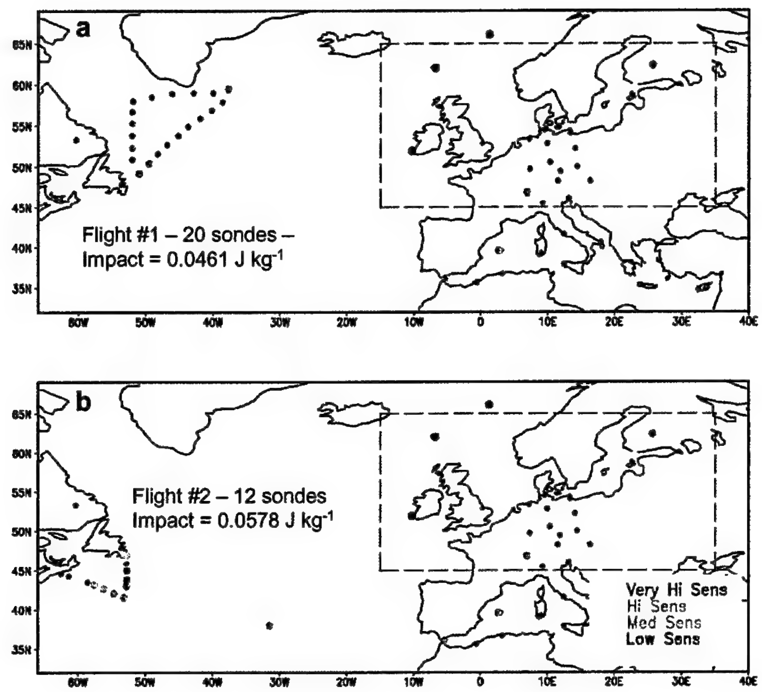

Figure 15: Estimated impact of two dropsonde configurations on the 42h NOGAPS forecast for northern Europe (area within red dash line). Targeted observing time is 18UTC 15 Nov 2003, forecast verification time is 12UTC 17 Nov 2003.

Fig. 15 illustrates the results of an observation sensitivity calculation for two possible targeting observing configurations involving dropsondes deployed by a reconnaissance aircraft. In this case, the targeted observing time is 18UTC 15 Dec 2003 and the forecast verification time is 12UTC 17 Dec 2003 (+42h). The forecast verification region is an area of the North Atlantic and northern Europe (indicated

by the dashed red box). The NOGAPS forecast trajectory used for the targeting calculations starts from an analysis at 00UTC 13 Dec 2003. Thus, in this example, there is a 66h "lead time" in which to produce the targeting guidance and deploy an aircraft to the target region. The costfunction (a proxy for the actual forecast error or forecast uncertainty) used here is the energy-weighted difference between two forecasts that verify at 12UTC 17 Dec 2003 - a 108h forecast from 00UTC 13 Dec 2003 and a 114h forecast from 18UTC 12 Dec 2003.

$$J_{t\,\mathrm{arg}} = \frac{1}{2} \langle \; (\mathbf{x}_{108} - \mathbf{x}_{114}) \; , \; \mathbf{C} \; (\mathbf{x}_{108} - \mathbf{x}_{114}) \rangle \; , \tag{17}$$

where $\mathbf{C}$ is a matrix of energy weighting coefficients for dry total energy (Rosmond 1997), and the NOGAPS forecast state vector $\mathbf{x}$ includes temperature, vorticity, divergence, and surface pressure. Note that for targeted observing, it is not known whether the desired outcome (a reduction in forecast error) corresponds to an increase or decrease in the value of the costfunction. An improved forecast might correspond to either an increase or decrease in forecast energy, or surface pressure over the verification region, for example. Thus, the impact function for targeted observing can only measure the expected impact of the observations in terms of a change in the variance or magnitude of J, under the assumption that if the observations have an impact on J there is also a potential for reduction in forecast error. One expression for the

expected impact of a configuration (n) of targeted observations is

$$|\delta J|_{(n)} = \left\langle \overbrace{\underbrace{|\mathbf{y} - \mathbf{H}\mathbf{x}_b|}_{\text{assumed innovation}}}^{regular\_obs}, \left|\frac{\partial J}{\partial \mathbf{y}}\right| \right\rangle + \left\langle \overbrace{\underbrace{|\mathbf{y} - \mathbf{H}\mathbf{x}_b|}_{\text{assumed innovation}}}^{t\arg eted\_obs}, \left|\frac{\partial J}{\partial \mathbf{y}}\right| \right\rangle . \quad (18)$$

Eq. (18) is a generalization of the observation impact equation (16) for the situation when the innovations and actual forecast errors are not known. Since the innovations are not known when the targeting guidance is prepared, it is necessary to use "assumed innovations" in (18). The assumed innovation can be, for example, an estimate of analysis uncertainty or background error, or even a constant, in which case $|\delta J|_{(n)}$ is directly proportional to the sensitivity gradient magnitude. In (18) both the "innovation" and the observation sensitivity appear as absolute values, so that each observation contributes to a positive value of $|\delta J|_{(n)}$. The total value of $|\delta J|_{(n)}$ is the inner product calculated over the global domain, including all regular and targeted observations.

In Fig 15a, Flight #1 is a set of 20 hypothetical dropsondes deployed from an altitude of 24,000 ft. The location of each dropsonde is indicated by a solid dot, and each dropsonde provides a vertical profile of temperature and wind on pressure surfaces at intervals of 100 mb, with the assumed accuracy of rawinsonde observations. Flight #2, shown in Fig. 15b, is a set of 12 hypothetical dropsondes with the same specifications as Flight #1. The other solid dots in Fig. 15 are locations of regular rawinsonde stations providing observations at the 18UTC time.

Observation Type	Control	Flight #1	Flight #2
Raobs	0.1520	0.1475	0.1483
Dropsondes	-	**0.0461**	**0.0578**
Satwinds	0.1560	0.1530	0.1536
Aircraft	0.3839	0.3794	0.3832
ATOVS	0.5003	0.4911	0.4894
Land Surface	0.0144	0.0143	0.0143
Ship Surface	0.0695	0.0690	0.0668
Total	**1.2761**	**1.3004**	**1.3134**

Table 3: Impact function $|\delta J|$ (J kg^{-1}) for targeted observing flight tracks shown in Fig. 15. Costfunction (J) is the energy-weighted difference between 108h and 114h forecasts verifying over Northern Europe at 12UTC 17 Dec. 2003.

Table 3 summarizes the targeting impact calculations using (18) with an assumed innovation of 1.0 and observation sensitivity calculated with the NAVDAS adjoint. With no dropsondes added, the value of $|\delta J|$ for this case is equal to 1.2761 J kg^{-1}. This number indicates the "potential" of the regular observing system to influence the forecast uncertainty represented by the costfunction. If no observations are assimilated, then $|\delta J| = 0$.

By adding various configurations of targeted observations, we can increase the potential impact of the total observing system. The 20 dropsondes in Flight #1 increase $|\delta J|$ to 1.3004 J kg^{-1} (Table 3). Note that adding the dropsondes decreases marginally the impact of other observation types, but increases the potential impact of

the total (regular + targeted) observing network, which is the desired result. Flight #2 includes only 12 dropsondes, but increases $|\delta J|$ to 1.3134 J kg^{-1} and is thus considered to be the better of the two possible dropsonde configurations. In fact, Flight #2 covers an area of stronger analysis sensitivity (not shown). This targeting example suggests a relatively modest forecast impact, changing $|\delta J|$ by approximately 2-3%. However, during the Winter Storm Reconnaissance Program (WSR) targeted dropsonde observations reduced short-range forecast errors by an average 10%-20% (Szunyogh et al. 2000) and by up to 50% over localized regions during the North Pacific Experiment (NORPEX, Langland et al. 1999).

An alternative equation to estimate the impact of targeted observations can be obtained (following Baker 2000) if we define J as the projection of the analysis error $\varepsilon_{\mathbf{a}}$ onto the analysis sensitivity gradient

$$\delta J = \varepsilon_a^T \frac{\partial J}{\partial \mathbf{x}_a} \ . \tag{19}$$

The expected variance of the change in the forecast aspect J is

$$\langle (\delta J)^2 \rangle = \left(\frac{\partial J}{\partial \mathbf{x}_a} \right)^T \langle \varepsilon_{\mathbf{a}} \varepsilon_{\mathbf{a}}^T \rangle \frac{\partial J}{\partial \mathbf{x}_a} \ , \tag{20}$$

where $\langle \varepsilon_{\mathbf{a}} \varepsilon_{\mathbf{a}}^T \rangle$ is the analysis error covariance matrix, given by

$$\mathbf{P}_a = \mathbf{P}_b - \mathbf{P}_b \mathbf{H}^{\mathrm{T}} \left(\mathbf{H} \mathbf{P}_b \mathbf{H}^{\mathrm{T}} + \mathbf{R} \right)^{-1} \mathbf{H} \mathbf{P}_b \ . \tag{21}$$

The second term in (21) represents the reduction of the background error covariance due to the presence of the observations. Eqs (20) and (21) can be combined

(Baker 2000), finally resulting in

$$\left\langle (\delta J)^2 \right\rangle = \left(\frac{\partial J}{\partial \mathbf{y}} \right)^T \left[\mathbf{H}\mathbf{P}_b\mathbf{H}^\mathbf{T} + \mathbf{R} \right] \frac{\partial J}{\partial \mathbf{y}} \,. \tag{22}$$

In (22) $\left\langle (\delta J)^2 \right\rangle$ is the expected reduction in the variance of δJ due to the targeted and regular observations. This expression can be evaluated using the observation sensitivity and "cob" vectors, both of which are provided by the NAVDAS adjoint.

4.5 Sensitivity to Observation Error

The quality of a data assimilation procedure depends partly on the specification of observation and background error. These error parameters are generally tuned or adjusted based on information from various sources, which may include values used in other data assimilation procedures or the results of forward "sensitivity" experiments in which specified errors are modified in more-or-less arbitrary ways. The trial and error sensitivity approach is generally an inefficient tuning procedure and is unlikely to produce the optimal specification of either observation or background error. For example, the results of conventional sensitivity tests are often ambiguous because the "tuning" generally produces a combination of positive and negative impacts that are partially self-canceling and conceal the actual potential for larger impact.

A potentially more efficient method of parameter tuning can use adjoint sensitivity information which, for a selected forecast costfunction, provides a complete sensitivity gradient vector for the entire observation space of the data assimilation procedure.

With this information, the specified observation errors (or other parameters) can be adjusted to achieve more optimal results with less trial and error.

The values of the observation error standard deviation $\varepsilon_{\mathbf{r}}$ in NAVDAS are specified by data statements in the innovation code module and written to the **innovation file**. In the NAVDAS adjoint code the **innovation file** is read and elements of the diagonal observation error covariance matrix $\mathbf{R}$ are defined as $r_i = (\varepsilon_{\mathbf{r}} \;/\; \varepsilon_{\mathbf{b}})^2$, where $\varepsilon_{\mathbf{b}}$ is the background error standard deviation at observation locations, and $\varepsilon_{\mathbf{b}}$ is used here as a normalization factor. We wish to obtain the sensitivity gradient $\partial J \;/\; \partial r_i$, which will be a vector in observation space. One method to obtain $\partial J \;/\; \partial r_i$ would be to write an adjoint (transpose) version of the discretized code that defines the NAVDAS operator $[\mathbf{HP}_b\mathbf{H^T} + \mathbf{R}]^{-1}$ in which $\varepsilon_{\mathbf{r}}$ and r_i appear. This has not been done because the operator is self-adjoint and additional adjoint code development was not necessary to obtain sensitivity to observations.

Alternatively, it is possible to define $\partial J \;/\; \partial r_i$ (the array *oberr_sens)* using variables already provided by the forward and adjoint versions of NAVDAS as

$$\frac{\partial J}{\partial r_i} = -\frac{\partial J}{\partial \mathbf{y}} * \mathbf{z} \;, \tag{23}$$

where $\mathbf{z}$ is the "cob" array defined by the solver in the forward NAVDAS ($\mathbf{z} = [\mathbf{HP}_b\mathbf{H^T} + \mathbf{R}]^{-1} (\mathbf{y} - \mathbf{Hx}_b)$). The NAVDAS adjoint reads $\mathbf{z}$ from the **rsd_vec file** and then computes $\partial J \;/\; \partial r_i$ after the calculation of $\partial J \;/\; \partial \mathbf{y}$ has been completed. The symbol (*) in (20) denotes a vector Shur product, not a vector inner or outer product. Note that

$\partial J \ / \ \partial r_i$ has the units of J, since r_i is non-dimensional. The array $\mathbf{z}$ obtained from the **rsd_vec file** has the units of $\mathbf{y}$. The derivation of (20) appears in Appendix C. This application of this sensitivity is currently under development.

5 Summary

A new adjoint code has been developed for the NRL Atmospheric Variational Data Assimilation System (NAVDAS), which performs a three-dimensional variational atmospheric analysis in observation space. The NAVDAS adjoint can be used to efficiently calculate the gradient of a forecast costfunction with respect to the complete vector of observations used for assimilation. In addition, sensitivity to the background and the specified observation error can be calculated. For the dry observed variables (temperature, wind, height), the observation sensitivity is shown to be accurate to within about 5% of the theoretical best-possible result. The error in this calculation is likely due to an inconsistency between the sensitivity to the NOGAPS initial surface pressure field and the NAVDAS analysis, which provides temperature and wind, but not an analyzed surface or sea-level pressure. At present, the NAVDAS adjoint does not include sensitivity to moisture observations, but it is configured for radiance assimilation (e.g., sensitivity to brightness temperature).

This report describes the main features of the NAVDAS adjoint, including key subroutines and the sequence of steps required to calculate observation sensitivity. The

main difference between the forward and adjoint versions of NAVDAS is the transposition of the post-multiplier $\mathbf{P}_b\mathbf{H}^\mathbf{T}$ from the forward NAVDAS into the operator $\mathbf{HP}_b$, which is used at the beginning of the NAVDAS adjoint sensitivity calculations.

The input for the NAVDAS adjoint is an analysis sensitivity vector, provided by the adjoint of a forecast model such as NOGAPS. A special interpolation procedure is required to transfer the analysis sensitivity from the NOGAPS grid onto the NAVDAS analysis grid. The NAVDAS adjoint uses the **innovation file** and the **rsd_vec file** produced by the regular (forward) NAVDAS procedure.

In Section 4, four examples of observation sensitivity applications are described: (i) simple examination of observation sensitivity gradients, (ii) impact of innovations on actual forecast error differences, (iii) sensitivity to hypothetical observations, and (iv) targeted observing. These examples illustrate the capability of the NAVDAS adjoint to provide sensitivity information for predictability studies and to study the performance of the data assimilation and quality control procedures.

References

Baker, N.L., 2000: Observation adjoint sensitivity and the adaptive observation-targeting problem. Ph.D. dissertation, Naval Postgraduate School, 265 pp [Available from the Naval Research Laboratory, 7 Grace Hopper Ave., Monterey, CA 93943.]

Baker, N. L., and R. Daley, 2000: Observation and background adjoint sensitivity in the adaptive observation targeting problem, *Q. J. R. Meteorol. Soc.*, **126**, 1431-

1454.

Bergot, T. and A. Doerenbecher, 2002: A study of the optimization of the deployment of targeted observations using adjoint-based methods. *Q. J. R. Meteorol. Soc.*, **128**, 1689-1712.

Bergot, T., G. Hello, and A. Joly, 1999: Adaptive observations: a feasibility study. *Mon. Wea. Rev.*, **127**, 743-765.

Buizza, R., J. Tribbia, F. Molteni, and T. Palmer, 1993: Computation of optimal unstable structures for a numerical weather prediction model. *Tellus*, **45A**, 388-407.

Daley, R., and E. Barker, 2001: *NAVDAS Source Book 2001.* NRL/PU/7530-01-441. Available from the Naval Research Laboratory, Monterey, CA 93943-5502, 163 pp.

Doerenbecher, A., and T. Bergot, 2001: Sensitivity to observations applied to FASTEX cases. *Nonlinear. Proc. Geophys.*, **8**, 467-481.

Errico, R.M., 1997: What is an adjoint model? *Bull. Amer. Meteor. Soc.*, **78**, 2577-2591.

Fourrie, N. A. Doerenbecher, T. Bergot, and A. Joly, 2002: Adjoint sensitivity of the forecast to TOVS observations. *Q. J. R. Meteorol. Soc.*, **128**, 2759–2777.

Gelaro, R., R. Buizza, T.N. Palmer, and E. Klinker, 1998: Sensitivity analysis and the construction of optimal perturbations using singular vectors. *J. Atmos. Sci.*, **55**, 1012-1037.

Guymer, L., 1978: Operational application of satellite imagery to synoptic analysis in the southern hemisphere. Tech. Report No. 26, Bureau of Meteorology, Melbourne, Australia.

Hogan, T. F., T. E. Rosmond, and R. L. Pauley, 1999: The navy operational global atmospheric prediction system: recent changes and testing of gravity wave and cumulus parameterizations. *Proc., 13th Conf. on Numerical Weather Prediction*, Denver, CO, Amer. Meteor. Soc., pp. 60-65.

Langland, R.H., and N.L. Baker, 2004: Estimation of observation impact using the NAVDAS adjoint system. *Tellus,* in-press.

Langland, R.H, and Coauthors, 1999: The North Pacific Experiment (NORPEX-98): Targeted observations for improved North American weather forecasts. *Bull. Amer. Meteor. Soc.*, **80**, 1363-1384.

Langland, R.H., R.L. Elsberry, and R. M. Errico, 1995: Evaluation of physical processes in an idealized extratropical cyclone using adjoint sensitivity. *Q. J. R. Meteorol. Soc.*, **121**, 1349–1386.

Langland, R. H., M. A. Shapiro, and R. Gelaro, 2002: Initial condition sensitivity and error growth in forecasts of the 25 January 2000 East Coast snowstorm. *Mon. Wea. Rev.*, **130**, 957-974.

Leutbecher, M., J. Barkmeijer, T.N. Palmer, and A.J. Thorpe, 2002: Potential improvement to forecasts of two severe storms using targeted observations. *Q. J. R.*

Meteorol. Soc., **128**, 1641–1670.

Palmer, T.N., R. Gelaro, J. Barkmeijer, and R. Buizza, 1998: Singular vectors, metrics, and adaptive observations. *J. Atmos. Sci.*, **55**, 633-653.

Rabier, F., E. Klinker, P. Courtier, and A. Hollingsworth, 1996: Sensitivity of forecast errors to initial conditions. *Q. J. R. Meteorol. Soc.*, **122**, 121-150.

Rao, P. A., C. S. Velden, and S. A. Braun, 2002: The vertical error characteristics of GOES-derived winds: description and experiments with numerical weather prediction. *J. Appl. Meteorol.*, **41**, 253-271.

Reale, A. L., M. L. Chalfant, A. S. Allegrino, F. H. Tiley, M. P. Gerguson and M. E. Pettey, 2003: Advanced-TOVS (ATOVS) sounding products from NOAA polar orbiting environmental satellites. *Proc., 12th Conf. on Satellite Meteorology and Oceanography*, Long Beach CA, 2003, paper JP1.15. Amer. Meteor. Soc.

Rosmond, T. E., 1997: *A Technical Description of the NRL Adjoint Modeling System.* NRL/MR/7532/97/7230. Available from the Naval Research Laboratory, Monterey, CA 93943-5502, 62 pp.

Szunyogh, I. and Coauthors, 2000: The effect of targeted dropsonde observations during the 1999 Winter Storm Reconnaissance Program. *Mon. Wea. Rev.*, **128**, 3520-3537.

Talagrand, O., and P. Courtier, 1987: Variational assimilation of meteorological observations with the adjoint vorticity equation. I: Theory. *Q. J. R. Meteorol. Soc.*,

113, 1311–1328.

Appendix A: Scripts and Code

Selected scripts, source codes and makefiles used to compile and run the NAVDAS adjoint are provided on the NRL computer **hadley** in the directory: /users_hadley/langland/NAVDAS_adjoint/. The NAVDAS adjoint currently runs on the SGI AMS cluster maintained by Fleet Numerical Meteorology and Oceanography Center. There are additional input and data look-up files located on AMS that are required to run the NAVDAS adjoint.

makefile

NAVDAS_adj.f (source code)

run_navdas_adjoint (c-shell script)

NAVDAS_adj.ksh (k-shell script)

gradtp.f (interpolation routine)

track.d1+t1_GIV_TRACK (targeted dropsonde input file)

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Appendix B: Derivation of Observation Impact Equation

Consider two nonlinear forecasts of lengths f and g both verifying at a time, t, for which there is a verifying analysis, $\mathbf{x}_t$. Forecast $\mathbf{x}_f$ is started from an analysis $\mathbf{x}_a$, and forecast $\mathbf{x}_g$ is started 6-h earlier (corresponding to the 6-h interval of the NAVDAS data assimilation cycle). The 6-h forecast of $\mathbf{x}_g$ provides the first-guess (or

background, $\mathbf{x}_b$) for the analysis $\mathbf{x}_a$ that represents the initial conditions for $\mathbf{x}_f$. The difference between the errors of forecasts $\mathbf{x}_f$ and $\mathbf{x}_g$ is given by $\Delta e_f^g = e_f - e_g$. We wish to derive expressions (or "impact functions") that can be used to estimate Δe_f^g using adjoint sensitivity gradients in both the gridpoint space of the forecast model and the observation space of the data assimilation procedure.

We first define quadratic measures of the two forecast errors using the expressions

$$e_f = \langle\ (\mathbf{x}_f - \mathbf{x}_t)\ ,\ \mathbf{C}\ (\mathbf{x}_f - \mathbf{x}_t)\rangle\ , \tag{B1}$$

$$e_g = \langle\ (\mathbf{x}_g - \mathbf{x}_t),\ \mathbf{C}\ (\mathbf{x}_g - \mathbf{x}_t)\rangle\ , \tag{B2}$$

where $\mathbf{C}$ is a matrix of energy weighting coefficients for dry total energy (Rosmond 1997). Using (B1) and (B2) we define two costfunctions

$$J_f = \frac{1}{2}\langle\ (\mathbf{x}_f - \mathbf{x}_t)\ ,\ \mathbf{C}\ (\mathbf{x}_f - \mathbf{x}_t)\rangle\ , \tag{B3}$$

$$J_g = \frac{1}{2}\langle\ (\mathbf{x}_g - \mathbf{x}_t),\ \mathbf{C}\ (\mathbf{x}_g - \mathbf{x}_t)\rangle\ , \tag{B4}$$

and the corresponding first derivatives

$$\frac{\partial J_f}{\partial \mathbf{x}_f} = \mathbf{C}\ (\mathbf{x}_f - \mathbf{x}_t)\ , \tag{B5}$$

$$\frac{\partial J_g}{\partial \mathbf{x}_g} = \ \mathbf{C}\ (\mathbf{x}_g - \mathbf{x}_t)\ . \tag{B6}$$

The true value of $e_f - e_g$, which we will call Δe_f^g, is defined as (B1) - (B2). We wish to have an expression for Δe_f^g that involves sensitivity gradients, and this can

be written using the gradients defined in (B5) and (B6) as

$$\Delta e_f^g = \left\langle (\mathbf{x}_f - \mathbf{x}_g) \, , \frac{\partial J_f}{\partial \mathbf{x}_f} + \frac{\partial J_g}{\partial \mathbf{x}_g} \right\rangle . \tag{B7}$$

It is easily shown that the RHS of (B7) is equivalent to the difference in forecast errors $e_f - e_g$. Note that it is necessary to use sensitivity gradients involving both the f and g trajectories because $e_f - e_g$ is the difference between two quadratic error expressions.

The difference between the forecast trajectories f and g at initial time is $\mathbf{x}_a - \mathbf{x}_b$, the analysis minus the background. If we assume that this initial difference evolves in a tangent linear sense into a good approximation of the forecast difference $\mathbf{x}_f - \mathbf{x}_g$, then we can estimate $e_f - e_g$ using $\mathbf{x}_a - \mathbf{x}_b$ and sensitivity gradients which the forecast model adjoint has mapped back to initial time along the two forecast trajectories. Thus, the adjoint model maps $\partial J_f \;/\; \partial \mathbf{x}_f$ into $\partial J_f \;/\; \partial \mathbf{x}_a$ along trajectory f and $\partial J_g \;/\; \partial \mathbf{x}_g$ is mapped into $\partial J_g \;/\; \partial \mathbf{x}_b$ along trajectory g, which allows us to write

$$\delta e_f^g = \left\langle \; (\mathbf{x}_a - \mathbf{x}_b) \, , \frac{\partial J_f}{\partial \mathbf{x}_a} + \frac{\partial J_g}{\partial \mathbf{x}_b} \right\rangle . \tag{B8}$$

Equation (B8) provides an estimate of $e_f - e_g$ in the gridpoint space of the forecast model. The result δe_f^g is not exact, although Δe_f^g in (B7) is exact, because the sensitivity gradients in (B8) are approximations obtained with the adjoint of NOGAPS. From (B8) we can derive an equivalent expression for δe_f^g in the observation space of the analysis procedure. First, we recognize from Eq. (6) in Section 2.2

that $\mathbf{x}_a - \mathbf{x}_b$ is equivalent to $\mathbf{K}\left(\mathbf{y} - \mathbf{H}\mathbf{x}_b\right)$, where the Kalman gain matrix $\mathbf{K} = \mathbf{P}_b\mathbf{H}^T \left[\mathbf{H}\mathbf{P}_b\mathbf{H}^T + \mathbf{R}\right]^{-1}$ (Daley and Barker, 2001). We may therefore re-write (B8) as

$$\delta e_f^g = \left\langle \mathbf{K}\left(\mathbf{y} - \mathbf{H}\mathbf{x}_b\right),\ \frac{\partial J_f}{\partial \mathbf{x}_a} + \frac{\partial J_g}{\partial \mathbf{x}_b} \right\rangle . \tag{B9}$$

Now, since $\mathbf{K}$ is linear, we can use the general definition of an adjoint operator $\langle \mathbf{K}\mathbf{y}\ ,\ \mathbf{x}\rangle = \langle \mathbf{y}\ , \mathbf{K}^T\mathbf{x}\rangle$ to write

$$\delta e_f^g = \left\langle \left(\mathbf{y} - \mathbf{H}\mathbf{x}_b\right),\ \mathbf{K}^T\left(\frac{\partial J_f}{\partial \mathbf{x}_a} + \frac{\partial J_g}{\partial \mathbf{x}_b}\right) \right\rangle . \tag{B10}$$

The operator $\mathbf{K}^T$ represents the adjoint of the data assimilation procedure, which defines a sensitivity gradient in observation space

$$\frac{\partial J_f^g}{\partial \mathbf{y}} = \mathbf{K}^T\left(\frac{\partial J_f}{\partial \mathbf{x}_a} + \frac{\partial J_g}{\partial \mathbf{x}_b}\right) . \tag{B11}$$

And using (B11) to substitute into (B10) we obtain (16) used in Section 4.2

$$\delta e_f^g = \left\langle \left(\mathbf{y} - \mathbf{H}\mathbf{x}_b\right),\ \frac{\partial J_f^g}{\partial \mathbf{y}} \right\rangle , \tag{B12}$$

which involves only observation space quantities. If there are no observations, then $\mathbf{x}_a = \mathbf{x}_b$ and $\delta e_f^g = 0$. The accuracy of the observation impact calculated in observation space (B12) is essentially equivalent to the gridpoint space calculation (B8).

Appendix C: Derivation of Sensitivity to Observation Error

The operator representing the solver step in the forward NAVDAS is

$$\mathbf{M} = [\mathbf{H}\mathbf{P}_b\mathbf{H}^{\mathbf{T}} + \mathbf{R}] \quad . \tag{C1}$$

Using $\mathbf{M}$ the "cob" vector ($\mathbf{z}$) is defined as

$$\mathbf{z} = \mathbf{M}^{-1}\,\mathbf{d} \quad , \tag{C2}$$

where $\mathbf{d}$ represents the innovation vector $(\mathbf{y} - \mathbf{H}\mathbf{x}_b)$. Next, (C2) is re-written as

$$\mathbf{M}\,\mathbf{z} = \mathbf{d}\;, \tag{C3}$$

and in perturbation form as

$$\delta\mathbf{M}\,\mathbf{z} + \mathbf{M}\,\delta\mathbf{z} = \delta\mathbf{d} \quad . \tag{C4}$$

In (C4) $\boldsymbol{\delta}\mathbf{z}$ represents perturbations of the "cob" vector, and $\delta\mathbf{M}$ represents perturbations of the $\mathbf{M}$ operator, which could include changes to the specified observation or background error covariance. Next, (C4) can be re-written as

$$\mathbf{M}\,\delta\mathbf{z} \;=\; \delta\mathbf{d} - \delta\mathbf{M}\,\mathbf{z} \quad , \tag{C5}$$

and,

$$\delta\mathbf{z} \;= \mathbf{M}^{-1}\,(\delta\mathbf{d} - \delta\mathbf{M}\,\mathbf{z}) \;\; . \tag{C6}$$

From (C6), and noting that $\mathbf{M}$ is self-adjoint, we obtain the following adjoint equations

$$\frac{\partial J}{\partial \mathbf{d}} = \mathbf{M}^{-1}\frac{\partial J}{\partial \mathbf{z}}\;, \tag{C7}$$

$$\frac{\partial J}{\partial \mathbf{M}} = -\mathbf{M}^{-1}\frac{\partial J}{\partial \mathbf{z}} * \mathbf{z} \ , \tag{C8}$$

where (*) denotes a vector Shur product. In (C7) the innovation sensitivity $\partial J \ / \ \partial \mathbf{d}$ is equivalent to $(\partial J \ / \ \partial \mathbf{y})$ if the background is not perturbed. We can thus substitute from (C7) into (C8) and obtain

$$\frac{\partial J}{\partial \mathbf{M}} = -\frac{\partial J}{\partial \mathbf{y}} * \mathbf{z} \ . \tag{C9}$$

The quantity $\partial J \ / \ \partial \mathbf{M}$ is a vector in observation space that represents the sensitivity of J with respect to the operator $\mathbf{M}$. Here, however, we are just concerned with sensitivity to the elements r_i of the observation covariance matrix $\mathbf{R}$. Then, assuming the operator $\mathbf{P_b}$ is not perturbed and since $\mathbf{R}$ is diagonal we obtain

$$\frac{\partial J}{\partial r_i} = -\frac{\partial J}{\partial \mathbf{y}} * \mathbf{z} \ , \tag{C10}$$

which is (23) in Section 4.5.